

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 181 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.02e-01

Confidence level: 7.33e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,3-Butadiene</div> <div>Measured: 274</div> <div>Predicted: 1100</div>	<div>Image not found</div> <div>Diethyl butanedioate</div> <div>Measured: 30.0</div> <div>Predicted: 7.43e-02</div>	<div>Image not found</div> <div>2-Methylpropanal</div> <div>Measured: 155</div> <div>Predicted: 123</div>
<div>Image not found</div> <div>Dodecylbenzene</div> <div>Measured: 317</div> <div>Predicted: 7.09e-05</div>	<div>Image not found</div> <div>Arecoline</div> <div>Measured: 232</div> <div>Predicted: 1.33e-01</div>	